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Ethylbenzene Production Case Study and Optimization

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ABSTRACT

Ethylbenzene Case Study and Optimization

(Under the direction of Dr. Adam Smith)

The objective of this project was to investigate the process of producing ethylbenzene from the liquid-phase reaction of ethylene and benzene and perform parametric and topological optimizations to increase the net present value of the production facility. To do so, the base case conditions of the process were modeled and quantified economically followed by an investigation into the existing process to determine conditions that could be altered to improve the economic viability of the project. After optimizing the parametric conditions and topology of the process, the net present value of the project was increased by 305 million dollars to 191 million dollars. In this process, ethylene and benzene are reacted in a continuous stirred-tank reactor to produce ethylbenzene, which is to be sold as a raw material to an adjacent styrene production facility. To model this process, the simulation software PRO/II was utilized so that the economic impact of changing process conditions and topology could be determined using an economic model created in Microsoft Excel. The operating conditions and equipment layout for the reactor, separations units, and utilities were investigated to determine the optimum operating conditions to maximize the net present value of the project. During this optimization portion, the PRO/II simulation was performed at various operating conditions for each area of interest in the process. The results of the economic model quantified the impact on net present value of the operating conditions for each of the simulation cases. This led to changes in the operating conditions in the reactor, phase separator, distillation columns, heat exchangers, and the compressor to identify the case that produced the maximum net present value.

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Project Introduction

The objective of this project was to perform a detailed case study on an ethylbenzene production unit and optimize the process to maximize its economic viability. The production process being investigated uses a liquid phase reaction scheme to convert 100 kmol/h each of pure ethylene and benzene into ethylbenzene via direct addition reaction. The ethylbenzene produced is to be sold to a styrene production plant. Our team modeled base case conditions given and then performed parametric and topological optimizations to increase the net present value of the project from negative 114 million dollars at the base case conditions to 191 million dollars.

The liquid phase production of ethylbenzene was achieved by reacting 100 kmol/h each of ethylene and ethylbenzene.

$$\underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{ethylbenzene}}{C_6H_5C_2H_5}$$

The side reaction between ethylene and ethylbenzene produces undesired diethylbenzene.

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{diethylbenzene}}{C_6H_4(C_2H_5)_2}$$

The third and final reaction occurs when diethylbenzene reacts with benzene to produce ethylbenzene.

$$\underset{\text{diethylbenzene}}{C_6H_4(C_2H_5)_2} + \underset{\text{benzene}}{C_6H_6} \rightarrow \underset{\text{ethylbenzene}}{2C_6H_5C_2H_5}$$

The feed streams entered the process at 1 atm and 25°C. The unreacted benzene exiting the reactor is separated from the other components and recycled to the fresh benzene feed. The liquid phase mixture exiting the phase separator is sent through a benzene tower that recovers 99.95% of benzene to the distillate and 99.9% of ethylbenzene to the bottoms. The bottoms from the benzene tower is fed to the ethylbenzene tower. The ethylbenzene tower recovers 99.9% of ethylbenzene to the distillate and 99.9% of diethylbenzene to the bottoms. Diethylbenzene byproduct will also be used as fuel. Ethylbenzene is obtained as a distillate from ethylbenzene tower and is sent to storage at 1 atm pressure and 50°C temperature. The base case process flow diagram is shown in the appendix A.

Certain basic economic parameters were considered for the economic analysis of the design. The design is for a grass-root facility to be developed on company's land over a period of 2 years starting from January 2022. Two-thirds of the equipment cost was allocated for the first year and one-third to the second year with a salvage value of 10% of the Fixed Capital Investment (FCI) at the end of the project life. The initial cost of buildings was assumed to be $1.0 M and the cost was distributed equally between the first and second year of construction and was assumed to be worth $0.5 M at the end of the project. Overall taxation rates were assumed to be 28% per year and the equipment depreciation was calculated under appropriate MACRS categories. Additionally, operating labor was priced at $77,800 per year per operator with 3% annual increase over the duration of the project. Pure ethylbenzene is priced at $900/tonne, pure benzene at $850/tonne, and ethylbenzene produced at $1935/tonne.

Base Case Analysis

This ethylbenzene production process was modeled using Pro/II simulation software. This allowed optimization to be performed by easily changing the base case parameters in the software and using the PRO/II generated data to calculate the economic metrics of the project. An economic model was also developed to calculate the net present value associated with the various costs and revenue from the PRO/II output data. The equipment costs were calculated using heuristics for sizing different types of equipment. As a result of these calculations, the equipment cost of the base case was concluded to be $15.1 M. The cost of the raw materials was then determined to be $76.3 M using the given prices of benzene and ethylene and the amount of both components that were needed to run this process. The annual revenue from the ethylbenzene product and off-gas streams was calculated to be $84.8 M. These costs and revenue were then put into an income and cash flow statement which ultimately finds the net present value. For this case study, we were looking at the net present value over a 12-year period. The net present value for the base case is -$114.2 M. The table below shows the values of the metrics previously discussed. The entire cash flow/income statement for the base case is shown in the appendix A.

Table 1: Economic Metrics for the Base Case

	Base Case
Annual Revenue	$ 84,810,216
Annual Cost of Materials	$ (76,261,560)
Total Cost of Equipment	$ (15,080,524)
NPV @ 12%	$ (114,194,747)

Pro/II can also calculate the single-pass conversion associated with a process. For this specific process, the conversion was at 49% for the base case. As well as conversion, Pro II can also calculate other reaction variables such as yield and selectivity.

Table 2: Process Metrics for the Base Case

Reaction Metrics	
Conversion	0.49
EB Yield	0.95
Selectivity to EB	35.31
EB Product FR (kmol/h)	46.40

When assessing the economic value of the project, it is important to figure out which economic components have the largest impact on the net present value by performing a sensitivity analysis. From the sensitivity analysis, the ethylbenzene revenue and the cost of raw materials had the largest impact on NPV, whereas the other costs (cost of labor, equipment, utilities) had a relatively small impact on the NPV. The price of the ethylbenzene and cost of material affected the NPV by over 200 million and the cost of labor, equipment and utilities affected the NPV by 8 to 15 million. These values were found based on a 60% variance window from the base case. This information is significant because the sale price of the ethylbenzene and the cost of the raw materials cannot be changed with optimization. However, the amount of ethylbenzene can be altered using optimization. Since the revenue of ethylbenzene relies on the price and flow rate of ethylbenzene, the percent change in the flow rate will affect the NPV the same as the price of ethylbenzene. For the optimization process, the goal is to optimize the flow rate of ethylbenzene so that more ethylbenzene can be produced, which will lead to a higher revenue and NPV. Based on this analysis of the base case, our team recommended moving forward with the project. The figure below shows the graph of the sensitivity analysis that was performed.

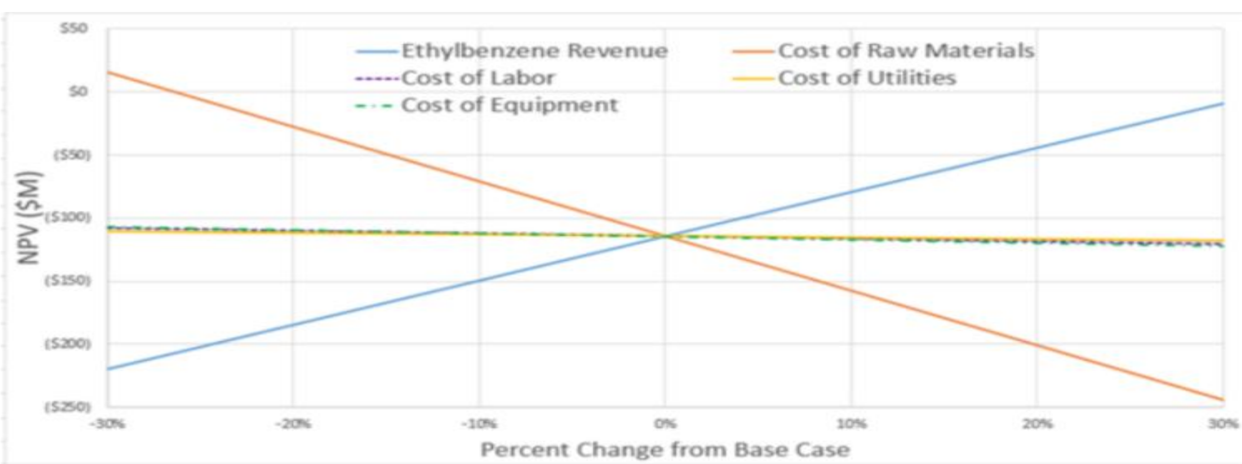


Figure 1: Base Case Sensitivity Analysis

Optimization

Upon analyzing the base case process, our team began parametric and topological optimization to improve the economic viability of the project through increasing the net present value. Following the design onion method, optimizations began with the reactor. After the reactor, the separations & recycle section were optimized followed by investigating the heat recovery system and the utilities. The team investigated each section by finding the parameters, or process conditions, that affected net present value and altered these until the maximum net present value was reached before moving to optimization of the next section. In some instances, changing the topological arrangement of the equipment was necessary to reach the maximum NPV. Based on the sensitivity analysis of the base case, the biggest opportunity for increasing NPV was by increasing the ethylbenzene production in the process by optimizing the process conditions.

Starting with the CSTR, the ethylbenzene produced by the reactor is a function of the rate of the reaction, or reaction kinetics, and the retention time, or the ratio of volume to volumetric flow rate. The reaction kinetics are largely a function of the temperature of the reaction with the rate of reaction generally increasing as temperature increases. As the volumetric flow rate of the reactants entering the reactor was not an independent variable but rather a function of the feed and recycle amount, the only way to change the retention time in the reactor was by changing the volume of the reactor. Thus, the team started the reactor optimization by altering the temperature of the reactor and plotting the NPV as a function of the temperature. The optimum reactor temperature was determined to be 85 °C with a maximum NPV of $17.5 M. The graph below shows this optimization. The increase in NPV was a result of the increased ethylbenzene production from 46.4 kmol/hr in the base case to 63.9 kmol/hr with the new reactor temperature.

This increase in production is attributable to the increase in conversion of ethylene in the reactor from 0.49 to 0.85 due to the increased rate of reaction at the higher temperature.

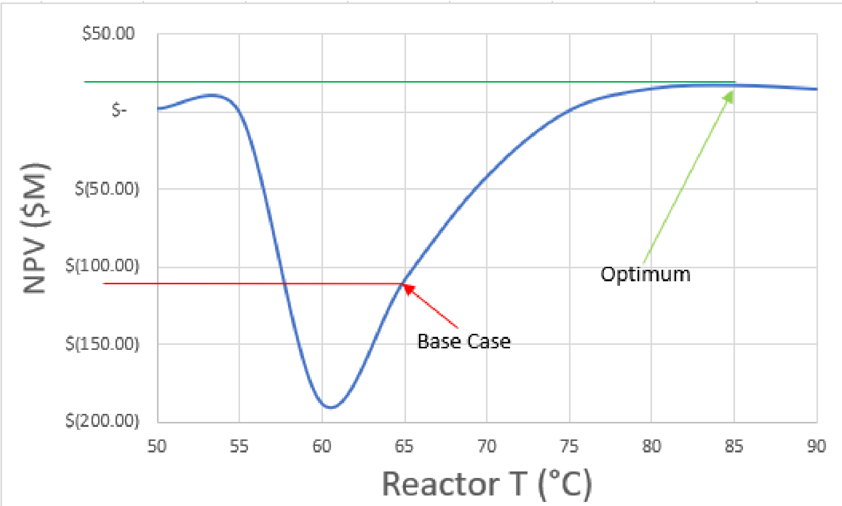


Figure 2: NPV vs Reactor Temperature (Iteration 1)

Following the optimization of temperature in the reactor, our team investigated changing the volume of the reactor to increase the retention time. However, after temperature had been optimized no additional NPV increase could be achieved by altering the reactor volume.

Next, the separations section and recycle were addressed beginning with the phase separator following the reactor. The two parameters that could be altered in the phase separator were the temperature and pressure. It was determined that increasing temperature and decreasing pressure in the phase separator from the 50 °C and 2 atm base case values would lead to increased ethylbenzene production. The purpose of the phase separator is to remove unreacted ethylene exiting the reactor to the off-gas stream. By removing the unreacted ethylene and recycling unreacted benzene, the selectivity of reaction series in the reactor is driven more to the production of ethylbenzene as opposed to the undesired product of diethylbenzene. The summary of the reaction kinetics that demonstrates this phenomenon is shown in the appendix C. By increasing the temperature and decreasing the pressure in the phase separator, a greater amount of ethylene exits the phase separator as vapor and is removed from the process before the distillation towers. This reduction in ethylene increases the relative percentage of benzene in the distillate of the first distillation tower, which decreases the vapor pressure of the distillate. At constant condenser conditions, this lower vapor pressure results in more of the benzene being condensed into the liquid recycle, which increases the concentration of benzene in the reactor. As previously mentioned, this increase in benzene concentration increases the selectivity of ethylbenzene production in the reactor. Investigating the temperature and pressure in the phase separator with respect to the optimum NPV yielded optimal values of 85 °C and 1.5 atm in the phase separator. These new temperature and pressure values increased the NPV from $17.5 M to $57.0 M. This increase in NPV is due to an increase in ethylbenzene production from 63.9 kmol/hr to 69.7 kmol/hr as a result of a selectivity increase from 6.1 to 11.2. The graphs demonstrating these optimization trials for temperature and pressure in the phase separator are shown below.

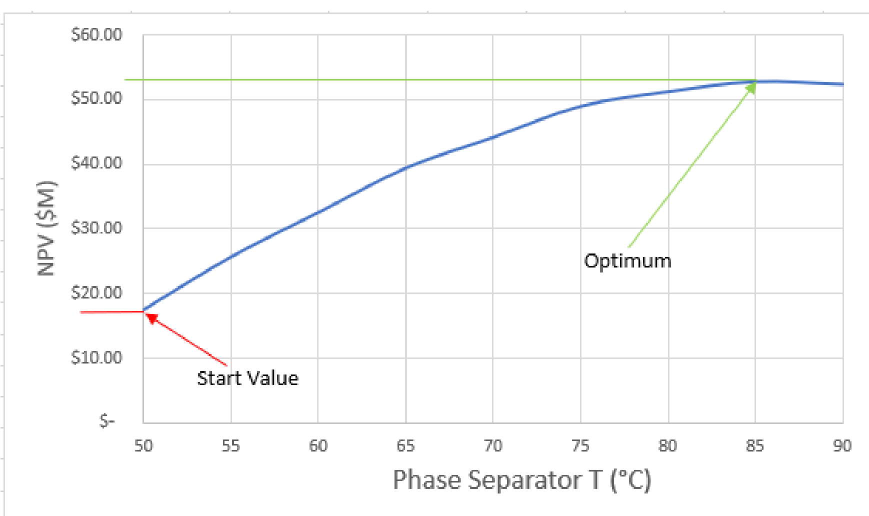


Fig 3: NPV vs Phase Separator Temperature

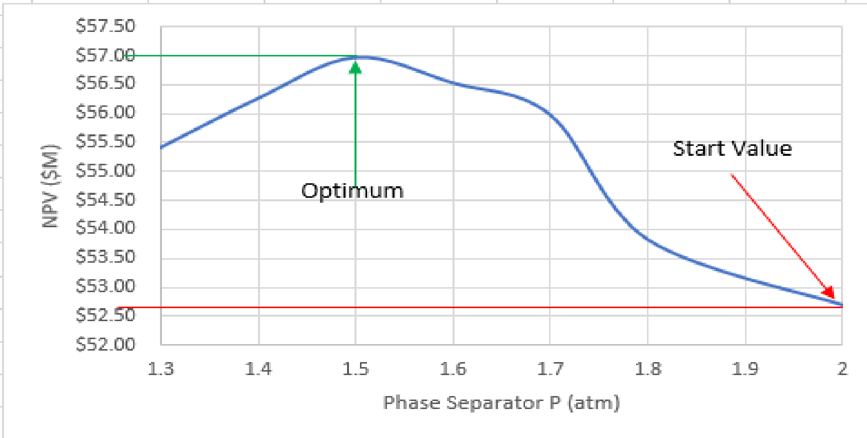


Fig 4: NPV vs Phase Separator Pressure

Following the phase separator, the next optimization was performed on the two distillation columns. The two parameters that could be changed in the towers to increase the NPV were pressure in the column and the feed tray location. The change in pressure and feed tray location had negligible impact on the ethylbenzene production in the process but did slightly increase the NPV through a reduction in utility costs by reducing the duty associated with the condenser and reboiler of each tower. The first optimization was moving the feed tray location in T-601 from location 13 to location 15, resulting in a $13,000 annual utilities savings. Next, the pressure in the condenser of T-602 was decreased from 1.2 atm to 1 atm, resulting in a $14,000 annual utilities savings. Finally, the feed tray location in T-602 was moved from location 10 to location 18 for a $57,000 annual utilities savings. These three optimizations increased the NPV from $57.0 M to $57.7 M. The graphs showing the trials leading the maximum NPV for each optimization are shown below.

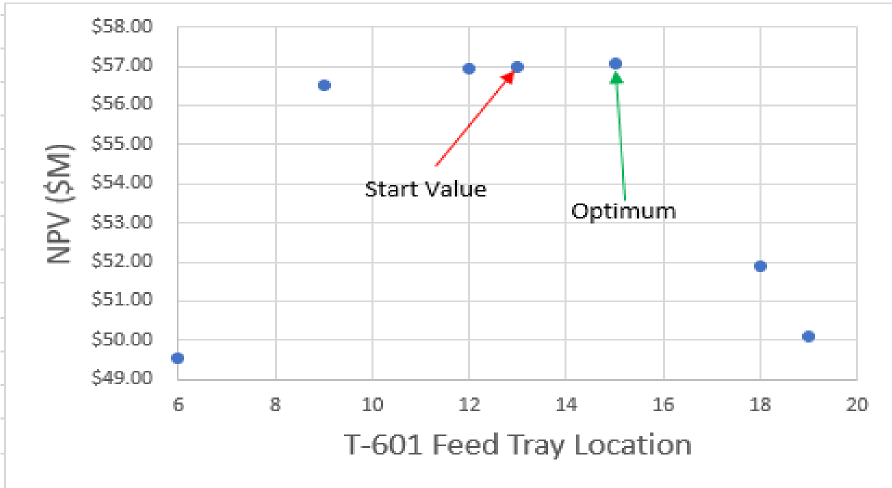


Fig 5: NPV vs T-601 Feed Tray Location

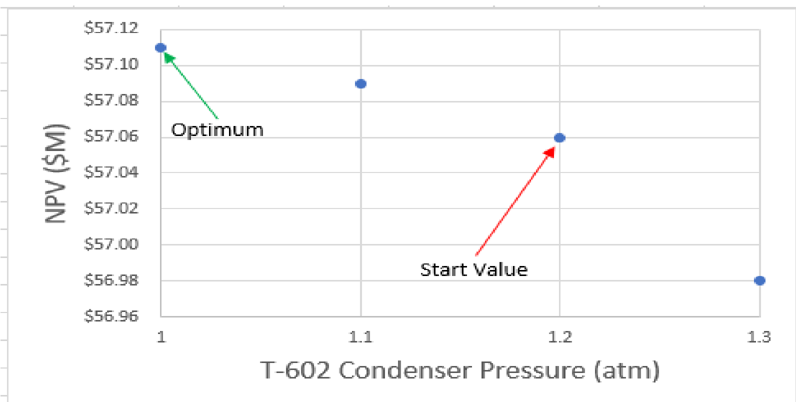


Fig 6: NPV vs T-602 Condenser Pressure

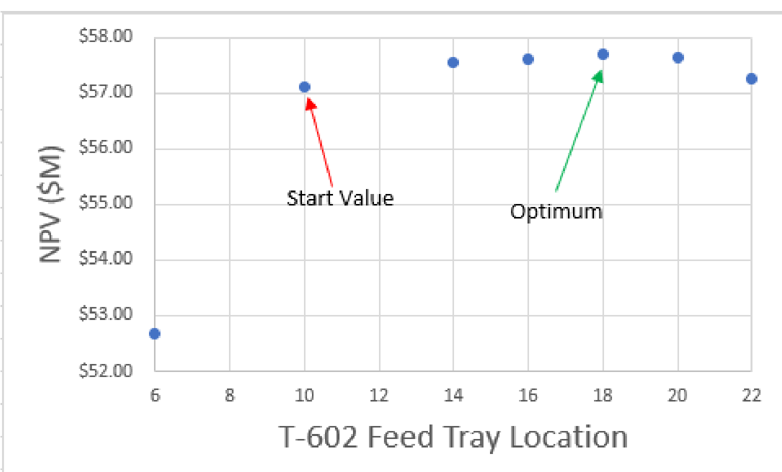


Fig 7: NPV vs T-602 Feed Tray Location

With the parameter optimizations made in the separations section, the benzene recycle entering the reactor increased by 120% compared to the amount of recycle present when the first reactor optimizations were performed. This significant change in benzene recycle allowed for a second iteration of reactor optimizations to further increase ethylbenzene production, so the temperature of the reactor was altered again with NPV being plotted at each temperature. This iteration found an optimum NPV value of $192 M at 155 °C in the reactor. This increase in NPV was a result of the increase of ethylene conversion to 0.99 and a resulting 94.4 kmol/hr of ethylbenzene being produced.

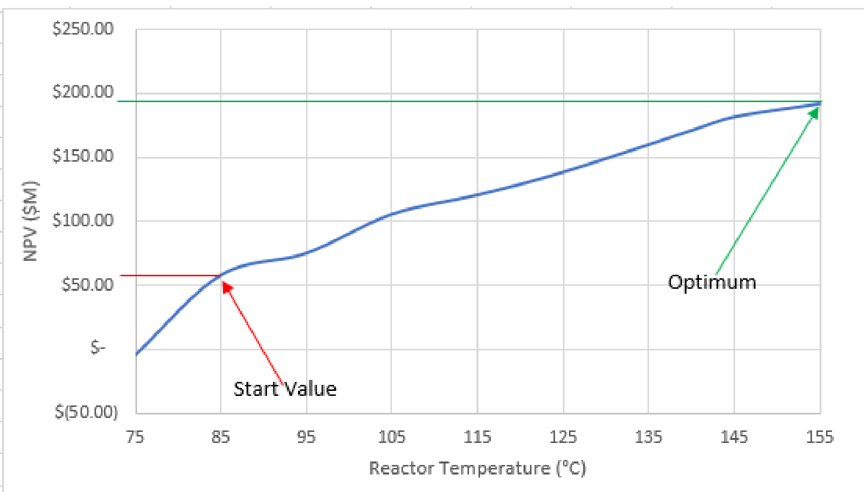


Fig 8: NPV versus Reactor Temperature (Iteration 2)

At a reactor temperature of 155 °C, the conversion of ethylene reached 0.99. This meant that the reactor effluent was entirely liquid and contained only 0.1% ethylene. As the purpose of the phase separator was to remove vapor, specifically ethylene, from the reactor effluent, the phase separator was no longer necessary. Thus, the phase separator and the heat exchanger (E-602) were removed from the process. This topological optimization reduced both equipment and utility costs and increased the NPV to $199 M.

The next step in the design onion optimization method was to investigate possible heat integration within the process to reduce equipment and utility costs. After the removal of E-602, the minimum number of heat exchangers was already achieved. This left the possibility of integrating E-601 and E-607 to reduce the utility costs associated with these heat exchangers. The potential utility savings from this integration was $5,000 per year. Our team deemed this integration to be unattractive due to the additional costs associated with the physical integration of these heat exchangers and the complications surrounding start-up. With E-607 being the ethylbenzene product heat exchanger, it would have no flow at start-up requiring utility streams to be connected to each heat exchanger. These additional costs and complications would outweigh the potential utility savings from the integration of the heat exchangers. Although no potential heat integrations opportunities are recommended within the ethylbenzene process, our team recommends investigating potential heat integration opportunities with the adjacent styrene process.

The final optimization that our team addressed was the ethylene compressor. In the base case, this compressor was a single compressor; however, at the new reactor conditions, the compression ratio this compressor was tasked with was 68:1. This is much higher than the optimal and feasible compression ratio of 3:1. Thus, the compressor system was staged using 4 compressors with intercoolers in between the first three compressors. This reduced the duty associated with compression from 551 kW to 429 kW. This would likely result in a less expensive compressor system. However, with the pricing correlations at our disposal and a conservative approach, the NPV was slightly decreased to $191 M. It should be noted that although the NPV was decreased, the process is not functional with the previous compressor design and quotes from equipment manufacturers should be less expensive than our team's estimation.

Optimized Design

Upon optimization, the benzene recycle was maximized leading to increased ethylene conversion and maximum ethylbenzene production. Additionally, we were able to eliminate two major pieces of equipment. The phase separator was no longer required as the reactor effluent was entirely liquid. We were also able to eliminate the heat exchanger that was located between the phase separator and the reactor. Along with that, our optimized design has a multistage compressor and intercooler system with 4 compressors that replace a previous compressor which was operating at an extremely high compression ratio. The annual revenue increased by 90% from $84 million per year to $161 million per year. Similarly, the NPV increased by over $300 million from negative $114 million to $191 million.

Optimization of the process also changed the reaction metrics. The single pass conversion of ethylene increased from 49% in base case to 99% in the optimized design. The flowrate of ethylbenzene in the product stream increased by about 103% from 46 kmol/h to 94 kmol/h. The significant change in reaction kinetics was a result of the increased reactor temperature and increased flowrate of benzene in the recycle stream.

The optimized design PFD and cash flow/income statement are shown in the appendix B.

Other Design Considerations

In the base case, all equipment was constructed using carbon steel. Upon review of the process including the expected corrosion, potential reactivity between carbon steel and the components in the process, and temperature in the process, our team recommends maintaining carbon steel construction of all equipment. As shown in the sensitivity analysis, the pricing of the raw materials and the ethylbenzene product significantly affect the economic value of the project. Moving forward in the design process, a dynamic economic model should be created to account for pricing fluctuations in the raw materials and ethylbenzene. This would give a more accurate estimation of the economic potential of the project. Additionally, it may not be feasible to obtain pure benzene and ethylene for the process. It is possible that slightly impure raw materials could be used to decrease the raw materials cost depending on the pricing. This would affect the ethylbenzene production in the reactor, as well as increase the required separations, but additional investigation should be performed to determine if impure ethylene and benzene could be used to increase the NPV of the project.

Safety Considerations

The most concerning safety hazard associated with this process is the high pressure surrounding reactor R-601. The streams going in and out of the reactor are operating at 68 atm and this could have some potential issues. Using high pressure conditions can lead to leaks or failures from connections and the reactor itself, especially in the event of a cooling jacket failure on the reactor. For this process, proper pressure relief valves need to be installed as well as control systems. Both of these implementations would promote an inherently safer design.

Recommendation

Based on our analysis, our team recommends moving forward with this project with our proposed optimizations. The process shows significant economic value with an NPV over $190 M. Table 3 on the following page shows the recommended optimizations in order of NPV impact.

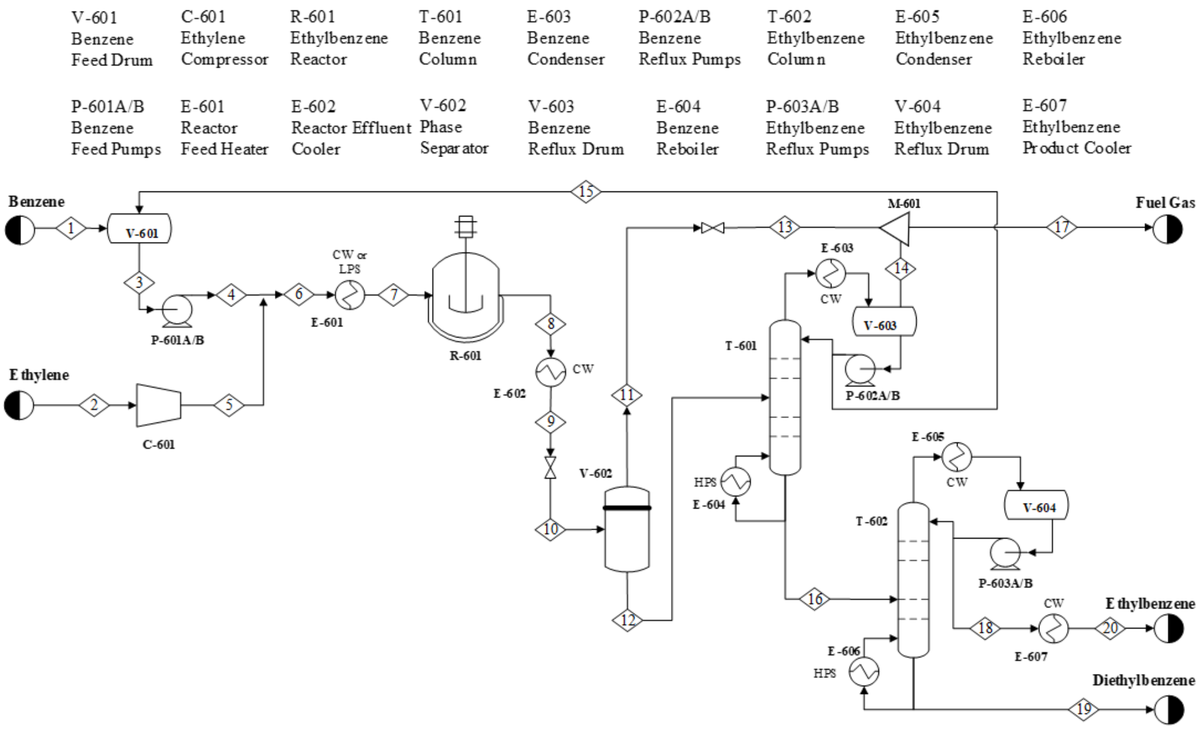
Table 3: NPV Impact by Optimization

Optimization	NPV Prior ($M)	NPV After ($M)	Increase in NPV ($M)
Reactor T from 85 ℃ to 155 ℃	$ 57.70	$ 192.40	$ 134.70
Reactor T from 65 ℃ to 85 ℃	$ (114.20)	$ 17.50	$ 131.70
Phase Separator T from 50 ℃ to 85 ℃	$ 17.50	$ 52.70	$ 35.20
Removal of E-602 and the Phase Separator	$ 192.40	$ 198.90	$ 6.50
Phase Separator P from 2 atm to 1.5 atm	$ 52.70	$ 56.97	$ 4.27
T-602 Feed Tray Location from 10 to 18	$ 57.10	$ 57.70	$ 0.60
T-601 Feed Tray Location from 13 to 15	$ 56.97	$ 57.06	$ 0.09
T-602 Condenser Pressure from 1.2 to 1.0 atm	$ 57.06	$ 57.10	$ 0.04
Staging of Compressor from 1 stage to 4 stages	$ 198.90	$ 191.30	$ (7.60)

Appendix

Appendix A: Base Case

A.1 Ethylbenzene Production Base Case PFD:



A.2 Base Case Stream Table:

Stream Name		S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	S20
Phase		Liquid	Vapor	Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid	Mixed	Vapor	Liquid	Vapor	Vapor	Liquid	Liquid	Vapor	Liquid	Liquid	Liquid
Temperature	°C	25.0	25.0	63.1	66.0	263.0	94.8	65.0	65.0	50.0	41.3	41.3	41.3	40.1	75.0	75.0	146.7	62.7	142.8	198.3	50.0
Pressure	ATM	1.0	1.0	1.0	39.3	39.3	39.3	39.1	39.1	38.9	2.0	2.0	2.0	1.0	1.0	1.0	1.3	1.0	1.2	1.5	1.0
Mole Fraction Vapor		0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.1	1.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0
Mole Fraction Liquid		1.0	0.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.9	0.0	1.0	0.0	0.0	1.0	1.0	0.0	1.0	1.0	1.0
Flow Rate	KG-MOL/HR	100.0	100.0	396.9	396.9	100.0	496.9	496.9	447.7	447.7	447.7	49.7	398.0	49.7	53.0	297.0	47.9	102.7	46.6	1.4	46.6
Benzene		100.0	0.0	396.5	396.5	0.0	396.5	396.5	348.7	348.7	348.7	6.0	342.7	6.0	45.8	296.7	0.2	51.8	0.2	0.0	0.2
Ethylbenzene		0.0	0.0	0.0	0.0	0.0	0.0	0.0	46.6	46.6	46.6	0.1	46.5	0.1	0.0	0.0	46.4	0.1	46.4	0.0	46.4
Ethylene		0.0	100.0	0.3	0.3	100.0	100.3	100.3	51.1	51.1	51.1	43.6	7.5	43.6	7.2	0.3	0.0	50.8	0.0	0.0	0.0
Diethylbenzene		0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	1.3	1.3	0.0	1.3	0.0	0.0	0.0	1.3	0.0	0.0	1.3	0.0

A.3 Base Case Equipment Summary:

Equipment Pricing Summary

CEPCI	2001	2016	Inflation	2022
	397.0	542.0	2.0%	610.4

EDS Row	Description	Equipment Size (A)		Equip Qty			C^0_P Tot ($\$_{2001}$)		F_P		F_M		F_q	F_{BM}		C^0_{BM}		C_{BM}	
		A			Spare				F_P	F_P Base	Figure A.18 F_i	F_M Base	F_q		F^0_{BM}	$C^0_{BM\text{-}2001}$ ($)		$C_{BM\text{-}2001}$ ($)	
Tag	Description	Tot Req	Purch ea	Base	Spares	Total	Each	Total	F_P	F^0_P	F_M	F^0_M	F_q	F_{BM}	F^0_{BM}	2001	2022	2001	2022
Heat Exchangers																			
E-601	Floating Hd	35.4	35.4	1	0	1	18,936	18,936	1.18	1.00	1.00	1.00	N/A	3.59	3.29	62,299	95,784	68,020	104,580
E-602	Floating Hd	32.1	32.1	1	0	1	18,710	18,710	1.18	1.00	1.00	1.00	N/A	3.59	3.29	61,556	94,640	67,179	103,286
E-603	Floating Hd	123.1	123.1	1	0	1	27,829	27,829	1.00	1.00	1.00	1.00	N/A	3.29	3.29	91,559	140,770	91,559	140,770
E-604	Kettle Reboiler	151.9	76.0	2	0	2	74,302	148,605	1.05	1.00	1.00	1.00	N/A	3.37	3.29	488,910	751,690	501,536	771,103
E-605	Floating Hd	15.5	15.5	1	0	1	18,595	18,595	1.00	1.00	1.00	1.00	N/A	3.29	3.29	61,178	94,060	61,178	94,060
E-606	Kettle Reboiler	31.5	31.5	1	0	1	36,497	36,497	1.05	1.00	1.00	1.00	N/A	3.37	3.29	120,076	184,614	123,177	189,382
E-607	Floating Hd	14.3	14.3	1	0	1	18,739	18,739	1.00	1.00	1.00	1.00	N/A	3.29	3.29	61,653	94,790	61,653	94,790
Vessels																			
V-601	Benzene Feed Drum	5.9	5.9	1	0	1	7,940	7,940	1.00	1.00	1.00	1.00	N/A	3.01	3.01	23,900	36,746	23,900	36,746
V-602	Phase Separator	12.4	12.4	1	0	1	13,049	13,049	1.00	1.00	1.00	1.00	N/A	4.07	4.07	53,110	81,655	53,110	81,655
V-603	Benzene Reflux Drum	5.8	5.8	1	0	1	7,914	7,914	1.00	1.00	1.00	1.00	N/A	3.01	3.01	23,822	36,625	23,822	36,625
V-604	EB Reflux Drum	1.7	1.7	1	0	1	4,421	4,421	1.00	1.00	1.00	1.00	N/A	3.01	3.01	13,308	20,460	13,308	20,460
Vessel Internals																			
VI-601		N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
VI-602	SS Demister	1.8	1.8	1	0	1	2,446	2,446	N/A	N/A	N/A	N/A	N/A	1.00	1.00	2,446	3,761	2,446	3,761
VI-603		N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
VI-604		N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Towers																			
T-601	Benzene Column	105.3	105.3	1	0	1	69,776	69,776	1.00	1.00	1.00	1.00	N/A	1.82	4.07	283,989	436,628	283,989	436,628
T-602	EB Column	27.6	27.6	1	0	1	23,231	23,231	1.00	1.00	1.00	1.00	N/A	1.82	4.07	94,552	145,371	94,552	145,371
Tower Internals																			
TI-601	Sieve Trays	5.0	5.0	34	0	34	3,148	107,019	N/A	N/A	N/A	N/A	1.00	1.00	1.00	107,019	164,540	107,019	164,540
TI-602	Sieve Trays	1.1	1.1	40	0	40	1,045	41,797	N/A	N/A	N/A	N/A	1.00	1.00	1.00	41,797	64,263	41,797	64,263
Reactors (towers)																			
R-601	Ethylbenzene Reactor	200.0	200.0	1	0	1	125,333	125,333	18.49	1.00	1.00	1.00	N/A	35.91	4.07	510,107	784,280	4,500,272	6,919,084
Pumps																			
P-601 A/B	Centrifugal	111.1	55.6	2	2	4	8,932	35,728	1.76	1.00	1.60	1.00	N/A	5.69	3.24	115,758	177,976	203,459	312,814
P-602 A/B	Included in T-601																		
P-603 A/B	Included in T-602																		
Pump Drives																			
PD-601 A/B	Elec Exp Proof	185.2	185.2	1	1	2	56,738	113,476	[redacted]					1.50	1.50	170,214	261,701	170,214	261,701
PD-602 A/B	Included in T-601																		
PD-603 A/B	Included in T-602																		
Compressor																			
C-601	Ethylene Compressor	458.6	458.6	3,000	459	1	152,369	152,369	0.00	0.00	N/A	N/A	N/A	1.00	2.70	411,397	632,516	411,397	632,516
Compressor Drives																			
CD-601	Elex Exp Proof	611.5	611.5	1	0	1	104,379	104,379	N/A	N/A	N/A	N/A	N/A	1.50	1.50	156,568	240,721	156,568	240,721
Heater(s)											F_T	F^0_T							
						Total		1,096,792							Total	2,955,217	4,543,591	7,060,155	10,854,856
															Rounded Up	2,956,000	4,544,000	7,061,000	10,855,000

Total Module (C_{TM})	C_{TM} = 1.18*C_{BM}	8,330,982	12,808,730
	Rounded Up	8,331,000	12,809,000
Grass Roots	C_{GR}/FCI=C_{TM}+0.5C^0_{BM}	9,808,591	15,080,524
	C_{GR}/FCI Rounded	9,809,000	15,081,000
	Bldg		1,000,000
	Land		-
	Total Investment		**16,081,000**

A.4 Base Case Cash Flow/Income Statement:

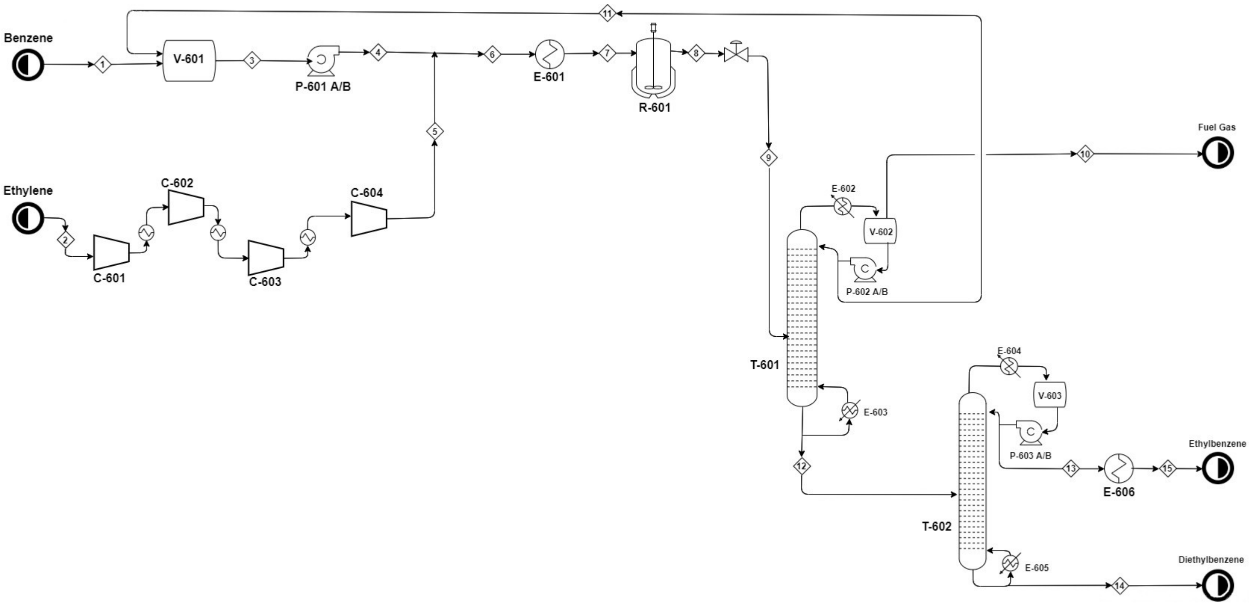
End of Year		-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
Income Statement																
Revenue					$84,810,216	$84,810,216	$84,810,216	$84,810,216	$84,810,216	$84,810,216	$84,810,216	$84,810,216	$84,810,216	$84,810,216	$84,810,216	$84,810,216
Expenses	Inflation															
Materials (C_{RM})	0%				(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)
Catalyst (C_{CF})	0%			-			-			-			-			
Labor (C_O)	3%				(1,478,200)	(1,522,546)	(1,568,222)	(1,615,269)	(1,663,727)	(1,713,639)	(1,765,048)	(1,817,999)	(1,872,539)	(1,928,715)	(1,986,576)	(2,046,173)
Utilities (C_{UT})	0%				(2,348,640)	(2,348,640)	(2,348,640)	(2,348,640)	(2,348,640)	(2,348,640)	(2,348,640)	(2,348,640)	(2,348,640)	(2,348,640)	(2,348,640)	(2,348,640)
Waste Treatment (C_{WT})	0%				-	-	-	-	-	-	-	-	-	-	-	-
Other (C_{OT})					(23,352,126)	(23,428,845)	(23,507,864)	(23,589,256)	(23,673,088)	(23,759,436)	(23,848,373)	(23,939,979)	(24,034,333)	(24,131,517)	(24,231,617)	(24,334,720)
Depreciation																
Land Depreciation					-	-	-	-	-	-	-	-	-	-	-	-
Land (BV)				$0	-	-	-	-	-	-	-	-	-	-	-	-
Building Depreciation					(24,573)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(24,573)
Bldg BV				$1,000,000	975,427	949,786	924,145	898,504	872,863	847,222	821,581	795,940	770,299	744,658	719,017	694,444
	MACRS Bldg				2.457265%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.457265%
Equipment Depreciation					(2,155,007)	(3,693,220)	(2,637,584)	(1,883,557)	(1,346,691)	(1,345,183)	(1,346,691)	(672,591)	-	-	-	-
Equipment BV				$15,080,524	12,925,517	9,232,297	6,594,713	4,711,156	3,364,465	2,019,282	672,591					
	MACRS Equp				14.29%	24.49%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%				
Taxable Income / (Loss)			-	-	(20,809,890)	(22,470,236)	(21,539,295)	(20,913,707)	(20,509,131)	(20,643,883)	(20,785,737)	(20,256,194)	(19,732,497)	(19,885,857)	(20,043,818)	(20,205,450)
Income Taxes	28%				5,826,769	6,291,666	6,031,003	5,855,838	5,742,557	5,780,287	5,820,006	5,671,734	5,525,099	5,568,040	5,612,269	5,657,526
Net Income / (Loss)				-	**(14,983,121)**	**(16,178,570)**	**(15,508,292)**	**(15,057,869)**	**(14,766,574)**	**(14,863,596)**	**(14,965,731)**	**(14,584,460)**	**(14,207,398)**	**(14,317,817)**	**(14,431,549)**	**(14,547,924)**
Cash Flow Statement																
Operating Activities																
Net Income / (Loss)		$0	$0	$0	(14,983,121)	($16,178,570)	($15,508,292)	($15,057,869)	($14,766,574)	($14,863,596)	($14,965,731)	($14,584,460)	($14,207,398)	($14,317,817)	($14,431,549)	($14,547,924)
Depreciation					2,179,580	3,718,861	2,663,225	1,909,198	1,372,332	1,370,824	1,372,332	698,232	25,641	25,641	25,641	24,573
Investment Activities																
Land																
Purchase		-														
Sale																-
Book Value																-
Taxable Gain/(Loss)																-
Taxes																
Net Gain/(Loss)																-
Net Cash Flow		-														-
Buildings																
Purchase			(500,000)	(500,000)												
Sale																500,000
Book Value																(694,444)
Taxable Gain/(Loss)																(194,444)
Taxes																
Net Gain/(Loss)																(194,444)
Net Cash Flow			(500,000)	(500,000)												500,000
Equipment																
Purchase			(10,053,683)	(5,026,841)												
Sale																1,508,052
Book Value																-
Taxable Gain/(Loss)																1,508,052
Taxes																
Net Gain/(Loss)																1,508,052
Net Cash Flow			(10,053,683)	(5,026,841)												1,508,052
Financing Activities																
Working Capital				(19,804,490)												19,804,490
Net Cash Flow		-	**(10,553,683)**	**(25,331,331)**	**(12,803,541)**	**(12,459,709)**	**(12,845,067)**	**(13,148,671)**	**(13,394,242)**	**(13,492,772)**	**(13,593,399)**	**(13,886,228)**	**(14,181,757)**	**(14,292,176)**	**(14,405,908)**	**7,289,191**
Cumulative Cash Flow		-	(10,553,683)	(35,885,014)	(48,688,555)	(61,148,264)	(73,993,331)	(87,142,002)	(100,536,244)	(114,029,016)	(127,622,415)	(141,508,643)	(155,690,400)	(169,982,576)	(184,388,484)	(177,099,292)
Payback Calc Conv																
PV @ S/U (12.0%MARR)		-	(11,820,125)	(25,331,331)	(11,431,733)	(9,932,804)	(9,142,865)	(8,356,218)	(7,600,253)	(6,835,858)	(6,148,963)	(5,608,415)	(5,114,084)	(4,601,698)	(4,141,354)	1,870,954
Cumul Discounted CF		-	(11,820,125)	(37,151,456)	(48,583,189)	(58,515,992)	(67,658,857)	(76,015,076)	(83,615,328)	(90,451,186)	(96,600,150)	(102,208,564)	(107,322,648)	(111,924,346)	(116,065,701)	(114,194,747)
Payback Calc Disc																

Summary Project Metrics		
MARR	**NPV @ (12.0%)**	**Payback (Conv)**
12.0%	**(114,194,747)**	Conv PB > 12
DCFROR	**AE(12.0%)**	**Payback (Disc @ 12%)**
#NUM!	(18,435,235)	Disc PB > 12

Appendix B: Optimized Design

B.1 Current Optimized Design PFD:

V-601 Benzene Feed Drum	C-601-604 Ethylene Compressors	R-601 Ethylbenzene Reactor	T-601 Benzene Column	E-602 Benzene Condenser	P-602 A/B Benzene Reflux Pumps	T-602 Ethylbenzene Column	E-604 Ethylbenzene Condenser
P-601 A/B Benzene Feed Pumps	E-601 Reactor Feed Heater	V-602 Benzene Reflux Drum	E-603 Benzene Reboiler	P-603 A/B Ethylbenzene Reflux Pumps	V-603 Ethylbenzene Reflux Drum	E-605 Ethylbenzene Reboiler	E-606 Ethylbenzene Product Cooler



B.2 Optimized Design Stream Table:

Stream Name		S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15
Phase		Liquid	Vapor	Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Mixed	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	°C	25.0	25.0	71.5	76.7	304.3	87.1	155.0	155.0	96.8	75.0	75.0	146.4	135.5	192.0	50.0
Pressure	ATM	1.0	1.0	1.0	68.3	68.3	68.3	68.1	68.1	1.5	1.0	1.0	1.3	1.0	1.3	0.8
Enthalpy	M*WATT	0.1	0.3	3.9	4.3	0.7	5.0	9.1	8.9	8.9	0.0	3.8	0.8	0.7	0.0	0.2
Molecular Weight		78.1	28.1	78.1	78.1	28.1	74.6	74.6	80.2	80.2	71.3	78.1	106.8	106.0	133.3	106.0
Mole Fraction Vapor		0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.3	1.0	0.0	0.0	0.0	0.0	0.0
Mole Fraction Liquid		1.0	0.0	1.0	1.0	0.0	1.0	1.0	1.0	0.7	0.0	1.0	1.0	1.0	1.0	1.0
Rate	KG-MOL/HR	100.0	100.0	1339.9	1339.9	100.0	1439.9	1439.9	1340.1	1340.1	1.2	1241.1	97.8	95.0	2.8	95.0
Benzene		100.0	0.0	1338.6	1338.6	0.0	1338.6	1338.6	1241.4	1241.4	1.1	1239.7	0.6	0.6	0.0	0.6
Ethylbenzene		0.0	0.0	0.1	0.1	0.0	0.1	0.1	94.6	94.6	0.0	0.1	94.5	94.4	0.1	94.4
Ethylene		0.0	100.0	1.3	1.3	100.0	101.3	101.3	1.4	1.4	0.2	1.3	0.0	0.0	0.0	0.0
Diethylbenzene		0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.7	2.7	0.0	0.0	2.7	0.0	2.7	0.0

B.3 Optimized Equipment Summary:

Equipment Pricing Summary

CEPCI	2001	2016	Inflation	2022
	397.0	542.0	2.0%	610.4

		Equipment Size (A)		Equip Qty			C^0_p Tot ($\$_{2001}$)		F_P		F_M		F_q	F_{BM}		C^0_{BM}		C_{BM}	
	Description	A			Spare				F_P	F_P Base	Figure A.18 F_M	F_M Base	F_q		F^0_{BM}	$C^0_{BM\,2001}$ ($)		$C_{BM\,2001}$ ($)	
Tag	Description	Tot Req	Purch ea	Base	Spares	Total	Each	Total	F_P	F^0_P	F_M	F^0_M	F_q	F_{BM}	F^0_{BM}	2001	2022	2001	2022
Heat Exchangers																			
E-601	Floating Hd	149.9	149.9	1	0	1	30,758	30,758	1.30	1.00	1.00	1.00	N/A	3.79	3.29	101,192	155,581	116,714	179,446
E-602	Floating Hd	485.2	485.2	1	0	1	69,878	69,878	1.00	1.00	1.00	1.00	N/A	3.29	3.29	229,897	353,463	229,897	353,463
E-603	Kettle Reboiler	322.2	80.5	4	0	4	78,641	314,565	1.05	1.00	1.00	1.00	N/A	3.37	3.29	1,034,919	1,591,169	1,061,646	1,632,260
E-604	Floating Hd	25.6	25.6	1	0	1	18,382	18,382	1.00	1.00	1.00	1.00	N/A	3.29	3.29	60,477	92,982	60,477	92,982
E-605	Kettle Reboiler	47.3	47.3	1	0	1	49,009	49,009	1.05	1.00	1.00	1.00	N/A	3.37	3.29	161,239	247,902	165,403	254,304
E-606	Floating Hd	28.0	28.0	1	0	1	18,478	18,478	1.00	1.00	1.00	1.00	N/A	3.29	3.29	60,792	93,467	60,792	93,467
Vessels																			
V-601	Benzene Feed Drum	19.8	19.8	1	0	1	15,784	15,784	1.00	1.00	1.00	1.00	N/A	3.01	3.01	47,511	73,047	47,511	73,047
V-602	Benzene Reflux Drum	24.8	24.8	1	0	1	18,167	18,167	1.00	1.00	1.00	1.00	N/A	3.01	3.01	54,683	84,075	54,683	84,075
V-603	EB Reflux Drum	3.1	3.1	1	0	1	5,847	5,847	1.00	1.00	1.00	1.00	N/A	3.01	3.01	17,599	27,059	17,599	27,059
Towers																			
T-601	Benzene Column	343.0	343.0	1	0	1	211,288	211,288	1.00	1.00	1.00	1.00	N/A	1.82	4.07	859,941	1,322,144	859,941	1,322,144
T-602	EB Column	45.9	45.9	1	0	1	34,614	34,614	1.00	1.00	1.00	1.00	N/A	1.82	4.07	140,880	216,600	140,880	216,600
Tower Internals																			
TI-601	Sieve Trays	16.2	16.2	34	0	34	13,004	442,125	N/A	N/A	N/A	N/A	1.00	1.00	1.00	442,125	679,758	442,125	679,758
TI-602	Sieve Trays	1.9	1.9	40	0	40	1,401	56,031	N/A	N/A	N/A	N/A	1.00	1.00	1.00	56,031	86,147	56,031	86,147
Reactors (towers)																			
R-601	Ethylbenzene Reactor	200.0	200.0	1	0	1	125,333	125,333	32.95	1.00	1.00	1.00	N/A	62.22	4.07	510,107	784,280	7,798,523	11,990,082
Pumps																			
P-601 A/B	Centrifugal	665.9	95.1	7	7	14	12,507	175,103	2.19	1.00	1.60	1.00	N/A	6.62	3.24	567,335	872,267	1,159,928	1,783,368
P-602 A/B	Included in T-601																		
P-603 A/B	Included in T-602																		
Pump Drives																			
PD-601 A/B	Elec Exp Proof	1109.8	1109.8	1	1	2	130,177	260,353						1.50	1.50	390,530	600,432	390,530	600,432
PD-602 A/B	Included in T-601																		
PD-603 A/B	Included in T-602																		
Compressor																			
C-601:604	Ethylene Compressor	429.1	450.0	4	0	4	144,297	577,187	0.00	0.00	N/A	N/A	N/A	1.00	2.70	1,558,405	2,396,018	1,558,405	2,396,018
Compressor Drives																			
CD-601	Elex Exp Proof	572.1	572.1	1	0	1	101,482	101,482	N/A	N/A	N/A	N/A	N/A	1.50	1.50	152,223	234,040	152,223	234,040
Heater(s)											F_T	F^0_T							
						Total		2,524,384							Total	6,445,887	9,910,431	14,373,309	22,098,692
															Rounded Up	6,446,000	9,911,000	14,374,000	22,099,000

Total Module (C_{TM})	$C_{TM} = 1.18{*}C_{BM}$	16,960,504	26,076,457
	Rounded Up	16,961,000	26,077,000
Grass Roots	C_{GR}/FCI=C_{TM}+0.5C^0_{BM}	20,183,448	31,031,671
	C_{GR}/FCI Rounded	20,184,000	31,032,000
	Bldg		1,000,000
	Land		-
	Total Investment		**32,032,000**

B.4 Optimized Design Utilities Summary

Utilities | Stream Time 8,322 h/yr | 95.000% Stream Factor

ID	Description	Utility	Rate (MJ/hr)	Price	In Units	Total Cost	Out Price	Out Units	Total Out	Net Utilities
Heat Exchangers										
E-601	Floating Hd	HPS	14,538	5.660	$/GJ	(684,771)				(684,771)
E-602	Floating Hd	CW	52,132	0.378	$/GJ	(163,992)				(163,992)
E-603	Kettle Reboiler	HPS	36,537	5.660	$/GJ	(1,720,990)				(1,720,990)
E-604	Floating Hd	CW	5,561	0.378	$/GJ	(17,494)				(17,494)
E-605	Kettle Reboiler	HPS	5,365	5.660	$/GJ	(252,692)				(252,692)
E-606	Floating Hd	CW	1,642	0.378	$/GJ	(5,166)				(5,166)
									Net HE Utilities	(2,845,105)

Reactor			Req Output (MJ/hr)	Efficiency	Req Input	Price			
R-601	CSTR	BFW	10799.64			0.378	$/GJ		(33,973)
								Cost of Reactor Utility	(33,973)

Pumps/Drives and Compressor Drives		Utility	Output (kW)	Efficiency	Input (kW)	Price			
PD-601 A/B	Elec Exp Proof	Electricity	1109.8	90%	1,233	0.0674	$/kW		(691,676)
PD-602 A/B	N/A								
PD-603 A/B	N/A								
									0
CD-601	Elex Exp Proof	Electricity	572.1	90%	636	0.0674	$/kW		(356,540)
								Cost of Electricity	(1,048,216)
Total Cost of Utilities									($3,927,294)

B.5 Optimized Design Cash Flow and Income Statement:

End of Year		-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
Income Statement																
Revenue					$161,219,016	$161,219,016	$161,219,016	$161,219,016	$161,219,016	$161,219,016	$161,219,016	$161,219,016	$161,219,016	$161,219,016	$161,219,016	$161,219,016
Expenses	Inflation															
Materials (C_{RM})	0%				(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)	(76,261,560)
Catalyst (C_{Cat})	0%			-			-			-			-			
Labor (C_{OL})	3%				(1,478,200)	(1,522,546)	(1,568,222)	(1,615,269)	(1,663,727)	(1,713,639)	(1,765,048)	(1,817,999)	(1,872,539)	(1,928,715)	(1,986,576)	(2,046,173)
Utilities (C_{UT})	0%				(3,927,294)	(3,927,294)	(3,927,294)	(3,927,294)	(3,927,294)	(3,927,294)	(3,927,294)	(3,927,294)	(3,927,294)	(3,927,294)	(3,927,294)	(3,927,294)
Waste Treatment (C_{WT})	0%				-	-	-	-	-	-	-	-	-	-	-	-
Other (C_{OT})					(26,586,423)	(26,663,142)	(26,742,161)	(26,823,553)	(26,907,385)	(26,993,733)	(27,082,670)	(27,174,275)	(27,268,630)	(27,365,814)	(27,465,914)	(27,569,016)
Depreciation																
Land Depreciation					-	-	-	-	-	-	-	-	-	-	-	-
Land (BV)				$0	-	-	-	-	-	-	-	-	-	-	-	-
Building Depreciation					(24,573)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(25,641)	(24,573)
Bldg BV				$1,000,000	975,427	949,786	924,145	898,504	872,863	847,222	821,581	795,940	770,299	744,658	719,017	694,444
MACRS Bldg					2.457265%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.564103%	2.457265%
Equipment Depreciation					(4,434,426)	(7,599,656)	(5,427,439)	(3,875,856)	(2,771,128)	(2,768,025)	(2,771,128)	(1,384,013)	-	-	-	-
Equipment BV				$31,031,671	26,597,245	18,997,589	13,570,150	9,694,294	6,923,166	4,155,141	1,384,013					
MACRS Equip					14.29%	24.49%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%				
Taxable Income / (Loss)			-	-	48,506,541	45,219,177	47,266,699	48,689,843	49,662,281	49,529,124	49,385,675	50,628,234	51,863,352	51,709,992	51,552,031	51,390,400
Income Taxes	28%				(13,581,831)	(12,661,370)	(13,234,676)	(13,633,156)	(13,905,439)	(13,868,155)	(13,827,989)	(14,175,906)	(14,521,739)	(14,478,798)	(14,434,569)	(14,389,312)
Net Income / (Loss)				-	**34,924,710**	**32,557,807**	**34,032,023**	**35,056,687**	**35,756,842**	**35,660,969**	**35,557,686**	**36,452,328**	**37,341,613**	**37,231,194**	**37,117,462**	**37,001,088**
Cash Flow Statement																
Operating Activities																
Net Income / (Loss)		$0	$0	$0	34,924,710	$32,557,807	$34,032,023	$35,056,687	$35,756,842	$35,660,969	$35,557,686	$36,452,328	$37,341,613	$37,231,194	$37,117,462	$37,001,088
Depreciation					4,458,999	7,625,297	5,453,080	3,901,497	2,796,769	2,793,666	2,796,769	1,409,654	25,641	25,641	25,641	24,573
Investment Activities																
Land																
Purchase		-														
Sale																-
Book Value																-
Taxable Gain/(Loss)																-
Taxes																
Net Gain/(Loss)																-
Net Cash Flow		-														-
Buildings																
Purchase			(500,000)	(500,000)												
Sale																500,000
Book Value																(694,444)
Taxable Gain/(Loss)																(194,444)
Taxes																
Net Gain/(Loss)																(194,444)
Net Cash Flow			(500,000)	(500,000)												500,000
Equipment																
Purchase			(20,687,781)	(10,343,890)												
Sale																3,103,167
Book Value																-
Taxable Gain/(Loss)																3,103,167
Taxes																
Net Gain/(Loss)																3,103,167
Net Cash Flow			(20,687,781)	(10,343,890)												3,103,167
Financing Activities																
Working Capital				(19,804,490)												19,804,490
Net Cash Flow		-	**(21,187,781)**	**(30,648,380)**	**39,383,709**	**40,183,104**	**39,485,303**	**38,958,184**	**38,553,611**	**38,454,635**	**38,354,455**	**37,861,982**	**37,367,254**	**37,256,835**	**37,143,100**	**60,433,318**
Cumulative Cash Flow		-	(21,187,781)	(51,836,161)	(12,452,452)	27,730,652	67,215,755	106,173,939	144,727,550	183,182,185	221,536,640	259,398,622	296,765,876	334,022,711	371,165,814	431,599,132
Payback Calc Conv						1.310										
PV @ S/U (12.0%MARR)		-	(23,730,315)	(30,648,380)	35,164,026	32,033,724	28,104,716	24,758,630	21,876,354	19,482,315	17,349,608	15,291,820	13,475,006	11,995,704	10,677,755	15,511,728
Cumul Discounted CF		-	(23,730,315)	(54,378,695)	(19,214,669)	12,819,055	40,923,772	65,682,402	87,558,756	107,041,071	124,390,679	139,682,498	153,157,505	165,153,208	175,830,963	191,342,691
Payback Calc Disc						1.600										

Summary Project Metrics		
MARR	**NPV @ (12.0%)**	**Payback (Conv)**
12.0%	**191,342,691**	1.310
DCFROR	**AE(12.0%)**	**Payback (Disc @ 12%)**
60.7%	30,880,753	1.600

Appendix C: Reaction Kinetics

The reaction kinetics are of the form:

$$-r_i = k_{o,i}\, e^{-E_i/RT}\, C_{ethylene}^{a} C_{EB}^{b} C_{benzene}^{c} C_{DEB}^{d}$$

where i is the reaction number above, and

i	E_i kcal/kmol	$k_{o,i}$	a	b	c	d
1	17,000	1.528×10^{6}	1	0	1	0
2	20,000	2.778×10^{7}	1	1	0	0
3	15,000	1,000	0	0	1	1

The units of r_i are kmol/s/m^3 of liquid phase, the units of C_i are kmol/m^3 and the units of $k_{o,i}$ vary depending upon the form of the equation.

Selectivity of Ethylbenzene:

$$S_{EB} = \frac{k_1 e^{\frac{-E_1}{RT}} C_E C_B - k_2 e^{\frac{-E_2}{RT}} C_E C_{EB} + k_3 e^{\frac{-E_3}{RT}} C_B C_{DEB}}{k_2 e^{\frac{-E_2}{RT}} C_E C_{EB} - k_3 e^{\frac{-E_3}{RT}} C_B C_{DEB}}$$

REFERENCES

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